SEMICLASSICAL TREATMENT OF THE DIRAC SEA CONTRIBUTION FOR FINITE NUCLEI

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ABSTRACT

Dirac sea corrections for bulk properties of finite nuclei are computed within a self-consistent scheme in the σ-ω model. The valence part is treated in the Hartree approximation whereas the sea contribution is evaluated semiclassically up to fourth order in $\hbar$. Numerically, we find a quick convergence of the semiclassical expansion; the fourth order contributing much less than one percent to the binding energy per nucleon.

PREPRINT UG-DFM-5/96

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1 Introduction

The quantum field theoretical approach to Nuclear Physics seems to be the only practical device known up to now to include relativistic corrections in the description of atomic nuclei in a systematic way [1, 2, 3, 4, 5]. In most works the description is limited to the valence part within a mean field Hartree approximation. Much less work has been devoted to the study of the Dirac sea of nucleons which should be included in principle to preserve the unitarity of the theory. The Dirac sea has been mostly considered in order to describe nuclear matter [3] or finite nuclei within the local density approximation up to two loops [6]. On the other hand, even at the lowest order of the loop expansion, the physical relevance of the single particle negative energy nucleon states in finite nuclei is not fully understood. The explicit inclusion of the sea presents both numerical and conceptual problems. A numerical computation of the Dirac sea energy would require the diagonalization of all the continuum states of the single particle Hamiltonian and subsequent renormalization. A more serious problem is represented by the appearance of short distance tachyonic ghosts in the meson propagators at the one loop level which makes the mean field vacuum state [7, 8] and nuclear matter [9] unstable against formation of translationally non-invariant configurations of size of the order of 0.2 fm. In the relativistic approach to Nuclear Physics, a prescription has recently been suggested to deal with the instability problem based on the Källen-Lehmann representation of two-point Green's functions which, so far, has only been applied to the study of nuclear matter and the corresponding local density approximation [10, 6]. In addition, the method presents ambiguities [11] and its extension to arbitrary Green's functions is not known.

A way out of the above mentioned difficulties, which applies specifically to the mean field approximation, is to treat the Dirac sea assuming that the mesonic mean fields are smooth functions in coordinate space, thus allowing for a derivative or semiclassical expansion of the Dirac sea contribution to the energy, but keeping the shell structure in the valence part. Indeed, the problem of the high momentum instability of the sea is circumvented since only low Euclidean momenta are probed by the semiclassical expan-

sion. Moreover, the numerical problems related to the continuum states or, equivalently, the non-local nature of the fermionic determinant, are drastically reduced to the study of an analytically given local functional of the mesonic fields and their lower derivatives. In fact, such an approach has been applied to compute the effect of the Dirac sea up to second order in $\hbar$ [7, 12]. There, it was found that such effects cannot be considered negligible. Obviously, there arises the question whether the higher order terms in the expansion can be safely neglected. There is, however, an additional subtlety, namely, even if the semiclassical expansion in powers of $\hbar$ turns out to be numerically convergent, there still could appear finite corrections of the type $\exp(-M_N Rc/\hbar)$ which might be numerically significant as compared to higher order $\hbar$ corrections. Such terms are beyond a semiclassical expansion and represent a sort of shell effects which, for the valence part, are known to be comparable to the second order $\hbar$ corrections [13]. Finally, an additional advantage of applying the semiclassical expansion to the Dirac sea lies in the absence of turning point divergences. In contrast, in the valence part these divergences take place and become a serious problem beyond second order, particularly in the formulation of a self-consistent approach.

In the present letter, we undertake the calculation of the fourth order term of the Dirac sea contribution to the binding energy per nucleon as well as other relevant observables. This is done in a combined self-consistent Hartree treatment of the positive energy single particle states and a semiclassical expansion of the negative energy states. For simplicity, we do so for the σ-ω model, although we expect our considerations to hold in more realistic versions including, e.g., ρ-meson as well as Coulomb interaction.

2 Field theoretical model

The σ-ω model is characterized by the following Lagrangian density [1]

$$
\begin{aligned}
\mathcal{L} = & \ \overline{\Psi}\left[\gamma_\mu(i\partial^\mu - g_v V^\mu) - (M - g_s\phi)\right]\Psi + \frac{1}{2}\left(\partial_\mu\phi\partial^\mu\phi - m_s^2\,\phi^2\right) + \\
& -\frac{1}{4}\,F_{\mu\nu}F^{\mu\nu} + \frac{1}{2}\,m_v^2 V_\mu V^\mu\,,
\end{aligned}
\tag{1}
$$

where Ψ is the isospinor nucleon field, ϕ the scalar field, V_μ the ω-meson field and $F_{\mu\nu} = \partial_\mu V_\nu - \partial_\nu V_\mu$. In the former expression the necessary counterterms

required by renormalization are implicitly included. In the time-independent mean field Hartree approximation the meson fields are replaced by classical c-numbers whereas the fermionic state is given by a Slater determinant consisting of valence plus sea single particle states. The total mean field energy is given by $E[\phi, V_0] = E^{\text{val}} + E^{\text{sea}} + E_B$, where

$$E^{\text{val}} = \sum_n E_n^{\text{val}}, \qquad E^{\text{sea}} = \sum_n E_n^{\text{sea}}$$

$$E_B = \frac{1}{2}\int d^3x \left[(\nabla\phi)^2 + m_s\phi^2 - (\nabla V_0)^2 - m_v V_0^2\right]. \qquad (2)$$

and the single particle valence and sea orbitals depend functionally on the mesonic fields ϕ and V_0 through the Dirac equation

$$[-i\alpha\cdot\nabla + g_v V_0(\mathbf{r}) + \beta(M - g_s\phi(\mathbf{r}))]\psi_n(\mathbf{r}) = E_n\,\psi_n(\mathbf{r})\,. \qquad (3)$$

Notice that in the nuclear ground state of spherical nuclei, the only case to be considered in this letter, the spatial components of the ω-meson field vanish [5].

To perform in practice the derivative expansion we borrow from refs. [14, 13], where the single particle level density $\rho(E)$ is obtained to fourth order in $\hbar$ for an arbitrary space dimension D. The sea energy can be deduced from eqs. (3) and (18) of ref. [14] by means of the relation

$$E^{\text{sea}} = \int_{-\infty}^0 dE\, E\, \rho(E)\,. \qquad (4)$$

The sea energy is ultraviolet divergent and requires a suitable renormalization. The standard dimensional regularization can be applied with $D = 3 - 2\epsilon$. Since we have in mind a semiclassical expansion of the sea energy we specify the renormalization conditions at zero momentum as done in ref. [5]. This results in the following expression for the renormalized sea energy to fourth order in the gradients of the mesonic fields

$$E_0^{\text{sea}} = -\frac{\gamma}{16\pi^2}M^4\int d^3\mathbf{r}\left\{\left(\frac{\Phi}{M}\right)^4\log\frac{\Phi}{M} + \frac{g_s\phi}{M} - \frac{7}{2}\left(\frac{g_s\phi}{M}\right)^2\right.$$
$$\left. +\frac{13}{3}\left(\frac{g_s\phi}{M}\right)^3 - \frac{25}{12}\left(\frac{g_s\phi}{M}\right)^4\right\}$$

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$$E_2^{\text{sea}} = \frac{\gamma}{16\pi^2} \int d^3\mathbf{r} \left\{ \frac{2}{3} \log \frac{\Phi}{M} (\nabla V)^2 - \log \frac{\Phi}{M} (\nabla \Phi)^2 \right\}$$

$$
\begin{aligned}
E_4^{\text{sea}} = \frac{\gamma}{5760\pi^2} \int d^3\mathbf{r} \Big\{ &- 11\,\Phi^{-4}(\nabla\Phi)^4 - 22\,\Phi^{-4}(\nabla V)^2(\nabla\Phi)^2 \\
&+ 44\,\Phi^{-4}((\nabla_i\Phi)(\nabla_iV))^2 - 44\,\Phi^{-3}((\nabla_i\Phi)(\nabla_iV))(\nabla^2V) \\
&- 8\,\Phi^{-4}(\nabla V)^4 + 22\,\Phi^{-3}(\nabla^2\Phi)(\nabla\Phi)^2 + 14\,\Phi^{-3}(\nabla V)^2(\nabla^2\Phi) \\
&- 18\,\Phi^{-2}(\nabla^2\Phi)^2 + 24\,\Phi^{-2}(\nabla^2V)^2 \Big\}.
\end{aligned}
\tag{5}
$$

Here, $V = g_v V_0$, $\Phi = M - g_s\phi$ and γ is the spin and isospin degeneracy of the nucleon, i.e., four if there are two nucleon species. The first two terms have been known for some time, see e.g. [5]. The fourth order term is new and turns out to be ultraviolet convergent. This was expected in advance since dimensional counting shows that there is a correspondence between the number of gradients and the superficial degree of divergence of the corresponding momentum integral.

3 Numerical results

The mean field equations of motion are obtained, as usual, by minimizing the total mean field energy functional, $E[\phi, V_0]$ (see definition above eq. (2)), with respect to arbitrary variations of $\phi(\mathbf{r})$ and $V_0(\mathbf{r})$. This yields eq. (3) together with

$$
\begin{aligned}
(\nabla^2 - m_s^2)\phi(\mathbf{r}) &= -g_s(\rho_s^{\text{val}}(\mathbf{r}) + \rho_s^{\text{sea}}(\mathbf{r})) \\
(\nabla^2 - m_v^2)V_0(\mathbf{r}) &= -g_v(\rho_v^{\text{val}}(\mathbf{r}) + \rho_v^{\text{sea}}(\mathbf{r}))
\end{aligned}
\tag{6}
$$

where we have explicitly separated the valence and sea contributions to the scalar and baryonic densities, $\rho_s = \langle \overline{\Psi}\Psi \rangle$ and $\rho_v = \langle \Psi^\dagger\Psi \rangle$, respectively. For both densities, the valence part is just the corresponding sum over valence orbitals. On the other hand, the sea densities can be obtained as

$$\rho^s(\mathbf{r}) = -\frac{1}{g_s}\frac{\delta E^{\text{sea}}}{\delta\phi(\mathbf{r})}, \qquad \rho^v(\mathbf{r}) = \frac{1}{g_v}\frac{\delta E^{\text{sea}}}{\delta V_0(\mathbf{r})}. \tag{7}$$

In turn, the expansion for E^{sea} given in eq. (5) provides a similar semiclassical expansion for the scalar and baryonic densities. We will consider closed-shell

nuclei for which the equations admit spherically symmetric solutions. These equations must be solved self-consistently. This poses no particular problems when the sea is included to zeroth or second orders since they give rise to second order differential equations. The fourth order case is qualitatively different since it requires to solve fourth order differential equations and consequently further boundary conditions need to be specified. Instead of doing so, the fourth order sea contributions are treated perturbatively, that is, we consider the full self-consistent solution to second order and use the resulting meson fields to compute the fourth order sea corrections to the binding energy and the nuclear radius. Obviously, due to the stationarity of the energy functional to second order, this procedure reproduces the correct fourth order correction to the energy up to higher order terms. As it will be shown below, the fourth order corrections turn out to be small, thus justifying *a posteriori* this procedure.

In Table 1 we present results for the binding energy per nucleon and mean squared charge radius for several closed-shell nuclei calculated in various approximations. In all cases, the parameters of the Lagrangian, namely, g_s, g_v, m_s and m_v, are adjusted to reproduce the ω-meson mass, the saturation density and binding energy per nucleon for nuclear matter and the mean squared charge radius of ^{40}Ca [2, 5]. The corresponding numerical values are given in Table 2. In both tables the entry "no sea" stands for the customary valence Hartree approximation, where the effects due to the Dirac sea are fully neglected. 0th- and 2nd-order represent the results of successive inclusion of the Dirac sea keeping the corresponding orders in the expression for the sea energy and sea densities in eqs. (5) and (7). The experimental values are given only for illustration, since the σ-ω model must be supplemented with additional degrees of freedom, such as the ρ-meson and Coulomb interaction, to be realistic [3, 5]. From Table 1, one can see that the Dirac sea corrections are not globally small and hence cannot be neglected. The effect becomes more dramatic on the fixing of the parameters, Table 2. Finally, in Table 3 we present our results for the full calculation where the Dirac sea is described semiclassically up to fourth order in $\hbar$. The various contributions to minus the total binding energy per nucleon are displayed, namely, valence kinetic energy, valence potential energy, minus sea potential energy and total sea energy. Their total sum yields minus the binding energy per nucleon.

In Table 1, the results for the fourth order have been intentionally omitted since they do not further modify the presented second order results. In fact, in

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all cases considered, i.e., closed-shell nuclei, the fourth order contributions are very small as they do not significantly influence neither the bulk properties nor the parameters of the model. The smallness of the correction does not follow from big cancelations of any kind; each term in eq. (5) turns out to be uniformly small in the integration region. This is an important result for it indicates that the semiclassical expansion converges much faster than one might naively expect. Indeed, the fourth order sea correction to the binding energy per nucleon can be estimated, from eq. (5), to be of the order of $1/(RA)$, R being the nuclear radius and A the mass number. In the case of calcium it corresponds to a correction of about 1 MeV. The fact that this number turns out to be much smaller is a direct consequence of the overall numerical dimensionless coefficient, whose value requires an explicit calculation, as done here. The higher orders are not expected to be relevant. For instance, the sixth order can be estimated to be suppressed by a further factor $1/(UR)^2$, U being the depth of either the scalar or the vector potentials, i.e., about one percent of the fourth order correction for calcium.

As already mentioned in the introduction, a word of caution is in order. The fast numerical convergence of the semiclassical expansion for the sea contribution to the mean field energy does not necessarily imply that it converges to the exact Hartree result. The expansion might be only asymptotic or it might be convergent but not to the exact result. Quite generally, non analytical terms in $\hbar$, which are beyond a semiclassical approach, are expected to occur in global properties. Actually, such contributions can be shown to appear in simple non relativistic quantum mechanical models [15]. The existence of these terms must be kept in mind if the semiclassical results are to be compared with an exact calculation, since they might introduce systematic deviations. Such deviations seem to have been observed in the quark chiral soliton model [16].

4 Conclusions

We summarize our points. The Dirac sea corrections to the mass and size of finite nuclei have been computed in a semiclassical self-consistent treatment of the σ-ω model, but taking into account the shell structure of the valence part by means of a Hartree approximation. In this combined self-consistent approach, we have investigated the numerical convergence of the semiclas-

sical expansion up to fourth order in $\hbar$ for the considered bulk properties. Although the Dirac sea as a whole cannot be considered negligible, the overall effect becomes smaller after the necessary readjustment of the parameters in the model. Furthermore, a fair description of the sea can be achieved by including just the zeroth and second order semiclassical terms. We emphasize the non triviality of this result since a simple dimensional estimate allows much larger corrections than the ones actually found at fourth order. Finally, the present calculations can be regarded as a previous step to an exact mean field description of the polarization of the Dirac sea.

Acknowledgments

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Table Captions

1. Binding energy per nucleon (in MeV) and mean squared charge radius (in fm) for closed-shell nuclei in successive calculational schemes. The "no sea" column stands for the purely valence calculation. The "sea 0th" and "sea 2nd" columns refer to inclusion of the sea through a semiclassical expansion. In all cases the parameters have been readjusted as explained in the main text. Experimental values are only given as orientative reference.

2. Parameters of the σ-ω model adjusted to fit the mean squared charge radius of ^{40}Ca and nuclear matter saturation density and binding energy (see ref. [3] for the definition of the parameters). The nucleon and ω meson masses are fixed to 939 MeV and 783 MeV respectively. The same calculational schemes as in the Table 1 are considered. The scalar meson mass is given in MeV.

3. In different columns, the valence kinetic energy, the valence potential energy, minus the sea potential energy and the total sea energy per nucleon are displayed for the full fourth order semiclassical approximation to the Dirac sea. Their total sum yields minus the binding energy per nucleon.

	No sea		Sea 0th		Sea 2nd		Exp.	
$^{A}_{Z}$X	B/A	m.s.c.r.	B/A	m.s.c.r.	B/A	m.s.c.r.	B/A	m.s.c.r.
$^{40}_{20}$Ca	6.28	3.48*	6.00	3.48*	6.33	3.48*	8.55	3.48
$^{48}_{20}$Ca	6.52	3.47	6.03	3.51	6.34	3.52	8.67	3.47
$^{56}_{28}$Ni	7.24	3.72	6.51	3.79	6.80	3.79	8.64	
$^{90}_{40}$Zr	8.36	4.22	7.99	4.23	8.22	4.25	8.71	4.27
$^{132}_{50}$Sn	8.81	4.60	8.43	4.66	8.62	4.68	8.36	
$^{208}_{82}$Pb	9.84	5.35	9.55	5.39	9.70	5.41	7.87	5.50

Table 1

	C_s^2	m_s	g_s	C_v^2	g_v
Nosea	357.741	449.93	9.06283	274.106	13.8056
Sea0th	227.840	368.37	5.92153	147.524	10.1281
Sea2nd	227.840	406.6	6.53607	147.524	10.1281

Table 2

$^{A}_{Z}$X	K$^{\text{val}}$	$-\frac{1}{2}\rho^{\text{val}}$ U	$\frac{1}{2}\rho^{\text{sea}}$ U	E$_0^{\text{sea}}$	E$_2^{\text{sea}}$	E$_4^{\text{sea}}$
$^{40}_{20}$Ca	14.6	-18.0	-5.29	1.68	0.681	$-2.6\cdot10^{-4}$
$^{48}_{20}$Ca	15.6	-18.8	-5.61	1.82	0.670	$8.3\cdot10^{-5}$
$^{56}_{28}$Ni	16.1	-19.5	-6.11	2.01	0.679	$6.7\cdot10^{-4}$
$^{90}_{40}$Zr	16.1	-20.3	-7.02	2.42	0.586	$-1.4\cdot10^{-5}$
$^{132}_{50}$Sn	16.7	-21.0	-7.52	2.66	0.526	$-1.0\cdot10^{-4}$
$^{208}_{82}$Pb	16.8	-21.7	-8.31	3.01	0.455	$-1.9\cdot10^{-4}$

Table 3